

Development of Novel Heterocyclic Compounds and Their Molecular Assemblies for Advanced Materials

Safety Office



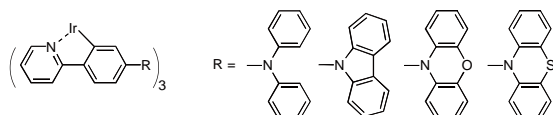
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Heterocycles containing sulfur and/or nitrogen atoms are useful as components of functional materials since heteroatoms in their rings are helpful to stabilize ions or ion-radical species, and extended π -conjugation decreases Coulombic repulsion. In addition intermolecular interactions caused by heteroatom contacts can be expected to form novel molecular assemblies. In this project new electron acceptors, donors, and donor-acceptor compounds based on heterocycles such as 1,2,5-thiadiazole and 1,3-dithiole were synthesized and their physical properties including those of the charge-transfer complexes or ion-radical salts were investigated. Unique crystal structures were constructed by using weak intermolecular interactions such as hydrogen bonding or heteroatom contacts.

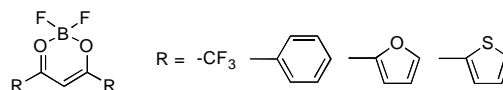
1. Synthesis and Electroluminescence Properties of *fac*-Tris(2-phenylpyridine)-iridium Derivatives Containing Hole-Accepting Moieties¹⁾

For effective organic electroluminescent (EL) devices, we synthesized *fac*-tris(2-phenylpyridine)iridium [Ir(ppy)₃] derivatives containing hole-trapping moieties, such as diphenylamine, carbazole, and phenoxazine. Their photoluminescent maxima were observed around the maximum of Ir(ppy)₃. These values were slightly shifted depending on the hole-trapping moieties. EL devices using an Ir complex with diphenylamine exhibited high EL performance because 1,1-bis[4-(di-*p*-tolylamino)phenyl]cyclohexane was employed as a hole-transporting layer. The maximum external quantum efficiency was recorded as 12.2% which is comparable to that observed in a device using Ir(ppy)₃.



2. Synthesis and Photoluminescence Properties of BF₂ Complexes with 1,3-Diketone Ligands²⁾

BF₂ complexes with 1,3-diketone ligands were synthesized, and their optical and electrochemical properties were studied. The colors of the complexes varied depending on the structures of the 1,3-diketone ligands. The absorption and emission maxima of the complexes with 1,3-diaryl-1,3-diketone ligands were considerably red shifted as compared to those of the complexes with 1-aryl-3-trifluoromethyl-1,3-diketone ligands, suggesting an extended p -conjugation of the 1,3-diaryl-1,3-diketone moieties. The molar absorption coefficients and quantum yields of the complexes with 1,3-diaryl-1,3-diketone ligands were larger than those of the complexes with 1-aryl-3-trifluoromethyl-1,3-diketone ligands. Cyclic voltammetry measurements revealed that the reduction potentials of the BF₂ complexes were higher than those of the free ligands. These complexes exhibited various emission colors in the solid states due to the intermolecular interactions.



References

- 1) K. Ono, M. Joho, K. Saito, M. Tomura, Y. Matsushita, S. Naka, H. Okada and H. Onnagawa, *Eur. J. Inorg. Chem.* 3676–3683 (2006).
- 2) K. Ono, K. Yoshikawa, Y. Tsuji, H. Yamaguchi, R. Uozumi, M. Tomura, K. Taga and K. Saito, *Tetrahedron* **63**, 9354–9358 (2007).